

SUBGRID MODELS FOR DRAG IN 3D GAS-PARTICLE FLOWS

USER MANUAL

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Revision Log

Version Number	Release Date	Description
Version 2015.10.0	10/31/2015	Fixed bugs in example files and updated user manual. Will be combined with other filtered models in future release.
Version 2015.03.0	3/31/2015	2015 initial release of package.

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To obtain support for this package, please send an email to
ccsi-support@acceleratecarboncapture.org.

1. INTRODUCTION

Resolution of small-scale structures such as particle clusters is computationally impractical for large-scale devices, especially when considering 3-dimensional (3D) models. The inability to resolve these small-scale structures results in erroneous simulation predictions.

To enable accurate macroscopic predictions using coarse-grid simulations, subgrid filtered models are developed. These filtered models account for the presence of unresolved physics via constitutive subgrid equations.

This product is an implementation of these subgrid models for gas-particle interphase drag in 3D flow in MFIX [1,2].

1.1. Motivating Example

Consider a bench-scale fluidized bed unit measuring 0.1 m in diameter by 0.4 m high, with solid-particles with a mean diameter (d_p) of 100 μm . Typically this system would be discretized into a fine-mesh with grid cells of $10 \times d_p = 1.0$ mm, resulting in a system of approximately 3.14 million cells. Alternatively, using a subgrid filtering approach and setting the (coarse) cell size to $50 \times d_p = 0.5$ cm results in a system of approximately 25,000 cells, a significant reduction.

2. INSTALLATION

These products do not require explicit installation; however, the user is required to have MFIX [1,2] made on their system to utilize the models. Note: These products were developed using source files from MFIX release 2014-1. Due to changes in the MFIX software structure, these models are not backwards compatible with previous MFIX releases, please use MFIX 2015-1.

2.1. System Requirements

This product requires MFIX [1-3].

2.2. Third Party Software

Open-source, multi-platform data analysis, and visualization application *ParaView* is recommend for post-processing of the MFIX simulation and can be downloaded from <http://paraview.org>. Other similar visualization software (for example, Tecplot, VisIt) can also serve the same purpose.

2.3. Product Usage

It is assumed that the user has built the required MFIX source files and created the entire MFIX directory, as detailed in [3].

To use the filtered models, ensure the following model files (found in `model`) are in the *local* run directory (in addition to the `mfix.dat` input file):

```
drag_gs.f
namelist.inc
run_mod.f
```

In addition to the standard MFIX keywords, the subgrid filtered models require the following keyword, as shown in Table 1.

Table 1: MFIX Keywords for the subgrid models.

SG_3D_HYDRO	LOGICAL
Flag for turning on/off the 3D hydrodynamics (drag) subgrid model. Requires the Wen-Yu drag model.	

Follow the MFIX instructions [3] to build the MFIX executable in the *local* run directory. Upon successful compilation, an `mfix.exe` executable is created in the *local* run directory.

3. EXAMPLE

An example input file for a cold-flow fluidized bed unit has been included with the release of this product to demonstrate implementation and use. This section describes the example.

3.1. Geometry

The geometry is based on the motivating example from Section 1.1. The domain measures 0.1 m in diameter by 0.4 m high. The bed is initialized as full ($EP_g = 0.41$) at a height of 0.155 m. There is mass-inflow of gas at the base that causes fluidization and a pressure outlet above the freeboard to equalize the pressure. The walls are set to no-slip boundary conditions.

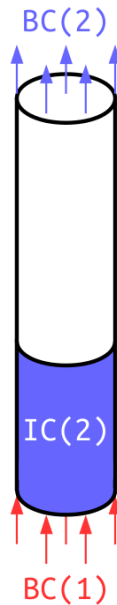


Figure 1: Schematics of bubbling fluidized bed example case, where BC denotes boundary conditions and IC denotes initial conditions. The blue IC(2) section represents the bed of solid particles.

3.2. Subgrid Model Settings

The subgrid model settings are as follows:

```
SG_3D_HYDRO = .TRUE.
```

3.3. Compiling and Running the Simulation

Recompile MFIX (as instructed in Section 2.3) using the following Bash commands:

1. `cd example/` # change directory to example/
2. `cp -r ../model/* .` # copy model files (recursively) to run directory, example/
3. `sh $MFIX/model/make_mfix` # make MFIX, recompile with local source files, where \$MFIX is the location of mfix/
4. `mpirun -np $NSLOTS mfix.exe` # execute simulation in parallel, where \$NSLOTS is the number of processors requested (i.e., NODESI*NODESJ*NODESK)

4. USAGE INFORMATION

4.1. Support

For technical support, send an email to ccsi-support@acceleratecarboncapture.org and/or fill out the “Submit Feedback/Request Support” form available on the product distribution page.

4.2. Restrictions

This model does not support multiple solid-phases and requires the use of the Wen-Yu drag model.

4.3. Next Steps

The future release will package the 3D gas-particle subgrid models with the 2D gas-particle-cylinder subgrid models.

5. DEBUGGING

Please refer to the following sections for debugging instructions and help contacts.

5.1. How to Debug

The constitutive drag model is implemented in `drag_gs.f`, while keywords are defined in `namelist.f` and `run_mod.f`. Debugging should mainly be within `drag_gs.f`.

5.2. Known Issues

There are no known issues at this time.

5.3. Reporting Issues

To report an issue, please send an email to ccsi-support@acceleratecarboncapture.org.

6. REFERENCES

- [1.] M. Syamlal, W. Rogers, T.J. O'Brien, MFIX Documentation Theory Guide. Technical Report, Department of Energy, National Energy Technology Laboratory.
- [2.] Multiphase Flow with Interphase eXchanges (MFIX). Available from <https://mfix.netl.doe.gov/>. Retrieved on October 31, 2015.
- [3.] MFIX User Guide. Available from <https://mfix.netl.doe.gov/>. Retrieved on October 31, 2015.